

Trifluoromethanesulfonic acid
1493-13-6 | DTXSID2044397

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.45e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.63e-01

Confidence level: 3.82e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Propene, 3-propoxy-</div> <div>Measured: 0.1</div> <div>Predicted: 64.5</div>	<div>Image not found</div> <div>Cyanamide</div> <div>Measured: 812</div> <div>Predicted: 8.50e-03</div>	<div>Image not found</div> <div>Decane</div> <div>Measured: 1.29</div> <div>Predicted: 1.26</div>
<div>Image not found</div> <div>Trichloroacetyl chloride</div> <div>Measured: 6.00e-02</div> <div>Predicted: 31.9</div>	<div>Image not found</div> <div>HFE-347pcf2</div> <div>Measured: 3.75e-03</div> <div>Predicted: 304</div>	